arXiv:1504.02968v1 [cond-mat.quant-gas] 12 Apr 2015

2DEG on a cylindrical shell with a screw dislocation

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Abstract

A two dimensional electron gas on a cylindrical surface with a screw dislocation is considered. More precisely, we investigate how both the geometry and the deformed potential due to a lattice distortion affect the Landau levels of such system. The case showing the deformed potential can be thought in the context of 3D common semiconductors where the electrons are confined on a cylindrical shell. We will show that important quantitative differences exist due to this lattice distortion. For instance, the effective cyclotron frequency is diminished by the deformed potential, which in turn enhances the Hall conductivity.

Keywords: 2DEG, Electron gas, Landau Levels, Hall Conductivity

1. Introduction

The influence of screw dislocations in quantum systems has received considerable attention over the last years. Some works are based on the geometric theory of defects in semiconductors developed by Katanaev and Volovich [1]. In this approach, the semiconductor with a screw dislocation is described by a Riemann-Cartan manifold where the torsion is associated to the Burgers vector. In this continuum limit, a screw dislocation affects a quantum system like an isolated magnetic flux tube, causing an Aharonov-Bohm (AB) interference phenomena [2]. The energy spectrum of electrons around this kind of defect shows a profile similar to that of the AB system [3–7]. These works describe the effect due to the geometric electron motion. A second ingredient, which may show pronounced influences in these quantum systems, is an additional *deformed potential* induce by a lattice distortion [8]. It is a repulsive scalar potential(noncovariant). The impact of this potential was first investigated in Ref. [9], where the scattering of electrons around a screw dislocation was investigated. Recently, it was showed that a single screw dislocation has profound influences on the electronic transport in semiconductors [10]. Both contributions, the covariant and noncovariant terms, were taken into account. Inspired in these works, in this paper, we will investigate how the deformed potential due to a lattice distortion affects the energy levels of a two dimensional electron gas (2DEG) confined on a cylindrical surface in a 3D semiconductor. The case with the absence of such potential described in the literature can find applications in the context of carbon nanotubes [11–13]. We will show that, for a 2DEG confined on a cylindrical shell in a 3D semiconductor like silicon, important quantitative differences exist due to this noncovariant term. The procedure to confine electrons on a curved surface is also considered, given rise to a geometric potential induced by such confinement [14].

This work is divided as follows. In Sec. 2, we derive the Schrödinger equation for a 2DEG on a cylindrical surface with the elastic deformation induced by the screw deslocation. In Sec. 3, we investigate how the deformed potential influences the energy levels of a 2DEG in the presence of an external magnetic field on such cylinder. This case can find applications in the context of quantum Hall effects, for instance. Next, we have the concluding remarks.

2. The Schrodinger equation for a 2DEG on the deformed cylinder

In this section, we derive the Schrodinger equation for the 2DEG on a cylinder with a deformation induced by a screw dislocation. We consider an infinitely long linear screw dislocation oriented along the z-axis. The three-dimensional geometry of the medium is characterized by a torsion which is identified with the surface density of the Burgers vector in the classical theory of elasticity. The metric of the medium with this kind of defect is given (in cylindrical coordinates) by [1]

$$ds^2 = (dz + \beta d\phi)^2 + d\rho^2 + \rho^2 d\phi^2, \tag{1}$$

In Eq. (1), $(\rho, \phi, z) \to (\rho, \phi + 2\pi, z)$ and β is a parameter related to the Burgers vector b by $\beta = b/2\pi$. The induced metric describes a flat medium with a singularity at the origin. The only non-zero component of the torsion tensor in this case is given by the two form

$$T^1 = 2\pi\beta\delta^2(\rho)d\rho \wedge d\phi, \tag{2}$$

with $\delta^2(\rho)$ being the two-dimensional delta function in the flat space. Figure 1 illustrates the formation of a screw dislocation in the bulk of a 3D crystal. We will consider an electron gas confined just on a cylindrical shell. Putting $\rho \equiv R =$ constant, the two dimensional line element will be given by

$$dl^2 = (dz + \beta d\phi)^2 + R^2 d\phi^2, \tag{3}$$

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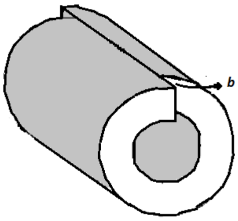

Figure 1: Cylindrical portion of a 3D solid showing the dislocation.

In Ref. [11], it was showed that the geometry of a cylindrical shell with a screw dislocation is equivalent to that of a cylindrical shell without a screw dislocation but with radius $r = \left(R^2 + \beta^2\right)^{1/2}$. This way, the line element 3 is rewritten as

$$dl^2 = dZ^2 + r^2 d\theta^2, \tag{4}$$

where

$$\theta = \phi + \frac{\beta Z}{r\sqrt{r^2 - \beta^2}}, \quad Z = \frac{z}{r}\sqrt{r^2 - \beta^2}. \tag{5}$$

This metric obeys the same usual identification, $(\theta, Z) \to (\theta + 2\pi, Z)$.

Unlike Ref. [11], which considers possible applications in the context of carbon nanotubes, we will consider common semiconductors. This way, we have to introduce a *deformed potential* which describes the effects of the lattice deformation on the electronic properties in such materials [8]. For a screw dislocation, it is found to be

$$V_d(\rho) = \frac{\hbar^2}{2ma^2}\frac{b^2}{4\pi^2\rho^2}\left[2 + a^2\left(\frac{\partial}{\partial z}\right)^2\right], \tag{6}$$

where a is the lattice constant.

We now consider the existence of a second quantum potential. The procedure to confine an electron gas on a surface is based on the Da Costa's approach [14]: we consider the charge carriers on a thin interface which is a infinity non flat quantum well. At the end, we consider the thickness of such interface going to zero and then we separate the transverse Schrodinger equation from the longitudinal one. In the transverse direction, the electrons are frozen due to the infinity quantum well, while they are free along the surface. The consequence is that a geometric potential arises. For electrons on a cylindrical surface, it is given by [14]

$$V_g(R) = -\frac{\hbar^2}{8mR^2}. \tag{7}$$

The Schrodinger equation for a quantum particle in a background $g_{\mu\nu}$ in the presence of both potentials described above is given by

$$-\frac{\hbar^2}{2m}\frac{1}{\sqrt{g}}\partial_\mu \sqrt{g}g^{\mu\nu}\partial_\nu\Psi + \left[V_d(R) + V_g(R)\right]\Psi = E\Psi, \tag{8}$$

where $g \equiv \det g_{\mu\nu}$. For a cylindrical shell with the metric 4, we have

$$-\frac{\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} + \frac{\partial^2}{\partial Z^2}\right]\Psi + \left[V_d(R) + V_g(r)\right]\Psi = E\Psi. \tag{9}$$

In the next section, we will consider the existence of a constant external magnetic field perpendicular to the cylinder height.

3. Landau levels of a 2DEG on a cylinder with screw dislocation

In this section, we investigate the influence of the deformed potential (6) on the energy levels of a 2DEG on a cylinder with a screw dislocation in common semiconductors. Since only the component of the magnetic field pointing along the surface normal governs the Lorentz force and the electronic transport in 2DEGs, we consider the presence of a uniform magnetic field crossing the cylinder transversely. Then, the vector potential in the symmetric gauge is

$$A_Z = Br\sin\theta. \tag{10}$$

This way, the Schrödinger equation in the background of Eq. (4) with such external magnetic field is [15]

$$-\frac{\hbar^2}{2mr^2}\frac{\partial^2\Psi}{\partial\theta^2} + \frac{1}{2m}\left[-i\hbar\frac{\partial}{\partial Z} - eA_Z\right]^2\Psi + \left[V_d(R) + V_g(r)\right]\Psi = E\Psi. \tag{11}$$

Since (6) depends on the linear momentum operator in the z-direction, we also considered the minimal coupling in it, $p_z \to p_Z - eA_Z$, together with the relation (5). Considering $\Psi = e^{ik_Z Z}\psi(\theta)$, the Schrödinger equation to be studied is

$$-\frac{\hbar^2}{2mr^2}\frac{\partial^2\psi}{\partial\theta^2} + \frac{m\omega_c^2}{2}\left(1 + \frac{\beta^2}{R^2}\right)^{-1}\left[r\sin\theta - \frac{\hbar k_Z}{eB}\right]^2\psi = \epsilon\psi, \tag{12}$$

where $\epsilon = E + \frac{\hbar^2}{8mR^2}\left(1 + \frac{\beta^2}{R^2}\right)^{-1} - \frac{\hbar^2\beta^2}{ma^2R^2}$. By defining the coordinate $x \equiv \theta/r$, we can rewrite Eq. (12) as

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{m\omega_c^2}{2}\left(1 + \frac{\beta^2}{R^2}\right)^{-1}\left[r\sin(x/r) - \frac{\hbar k_Z}{eB}\right]^2\psi = \epsilon\psi. \tag{13}$$

Considering the approximation for a sufficiently strong normal to the surface component of the magnetic field and for electrons with the Landau oscillator suspension center far enough from the side edges of a cylindrical strip, we expand the potential present in Eq. (13) around the minimum $x_M = r\sin^{-1}(\hbar K_Z/eBr)$ up to the harmonic term. The result of this operation provides us the following eigenvalue equation:

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{m\omega^2}{2}\left[x - x_M\right]^2\psi = \epsilon\psi. \tag{14}$$

with the effective cyclotron frequency

$$\begin{aligned}\omega &\equiv \omega_c\left(1 + \frac{\beta^2}{R^2}\right)^{-\frac{1}{2}}\cos\left[\sin^{-1}\left(\frac{\hbar k_Z}{eBr}\right)\right], \\ &= \omega_c\left(1 + \frac{\beta^2}{R^2}\right)^{-\frac{1}{2}}\sqrt{1 - \left(\frac{\hbar k_Z}{eBr}\right)^2}.\end{aligned} \tag{15}$$

Notice that $\omega < \omega_c$.

The eigenvalues of Eq. (14) are the Landau levels and the energy levels are

$$\begin{aligned} E_n &= \left(n+\frac{1}{2}\right)\hbar\omega_c\left(1+\frac{\beta^2}{R^2}\right)^{-\frac{1}{2}}\sqrt{1-\left(\frac{\hbar k_Z}{eBr}\right)^2} \\ &- \frac{\hbar^2}{8mR^2}\left(1+\frac{\beta^2}{R^2}\right)^{-1}+\frac{\hbar^2}{m}\frac{\beta^2}{a^2R^2}. \end{aligned} \tag{16}$$

For $\beta \rightarrow 0$, we have [16]

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega_c\sqrt{1-\left(\frac{\hbar k_z}{eBR}\right)^2}-\frac{\hbar^2}{8mR^2},$$

while that for $R \rightarrow \infty$, we have the Landau levels for electrons on a flat sample. Considering $b/a = 1$[17] and defining the dimensionless parameters $q \equiv rk_Z = Rk_z$, $\alpha \equiv 2eBR^2/\hbar$ and $\lambda^2 \equiv \beta^2/R^2$, we put Eq.(16) in the following form:

$$\begin{aligned} \frac{2mR^2E_n}{\hbar^2} &= \left(n+\frac{1}{2}\right)\alpha\left(1+\lambda^2\right)^{-\frac{1}{2}}\sqrt{1-4\left(\frac{q^2}{\alpha^2}\right)} \\ &- \frac{1}{4}\left(1+\lambda^2\right)^{-1}+\frac{1}{4\pi^2}. \end{aligned} \tag{17}$$

In the absence of the deformed potential, the energy of the system is [13]

$$\frac{2mR^2E'_n}{\hbar^2} = \left(n+\frac{1}{2}\right)\alpha\sqrt{1-4\left(\frac{q^2}{\alpha^2}\right)}-\frac{1}{4}\left(1+\lambda^2\right)^{-1}. \tag{18}$$

From this expression, we can see how the presence of a deformed potential has a pronounced influence since when it is absent, the Landau levels are just shifted by the geometric potential. In Figs. 2, 3 and 4, we evaluate the difference between these two cases given by Eqs. (17) and (18). We plot the energy difference which is $\Delta = \left|E_n - E'_n\right|$. In Fig. 2, we have the energy difference versus Rk_z. The maximum difference is at $k_z = 0$. This figure shows that, unlike the case of a 2DEG on a flat sample, the Landau levels are not dispersionless. In Fig. 3, we can see that the difference between the two spectra is pronounced as the ratio between the Burgers vector and the radius of the cylinder is increased. The energy difference versus the magnetic field is provided in Fig. 4. It can be seeing that it is increased as the magnetic field intensity is increased. There is a value of the magnetic field for which $\Delta = 0$. After examining the influence of the deformed potential due to lattice distortions, we now analyze how the screw dislocation affects the energy levels in comparison to the case of a flat sample.

In Fig. 5, we plot the dispersion curves, that is, E_n versus Rk_z for different values of the magnetic field. The curves are also equally spaced and the maximum values of energy are lower than the Landau levels in a flat sample. In Fig. 6 we investigate how the screw dislocation affects the ground state energy, $n = 0$. We consider different values of the magnetic field. Notice that, when $\beta/R = 0$, there is still the geometric potential (7) due to curvature and for this reason the energy levels are lower than in the case of a flat sample. Finally, in Fig. 7, the energy levels are depicted as function of magnetic field. For

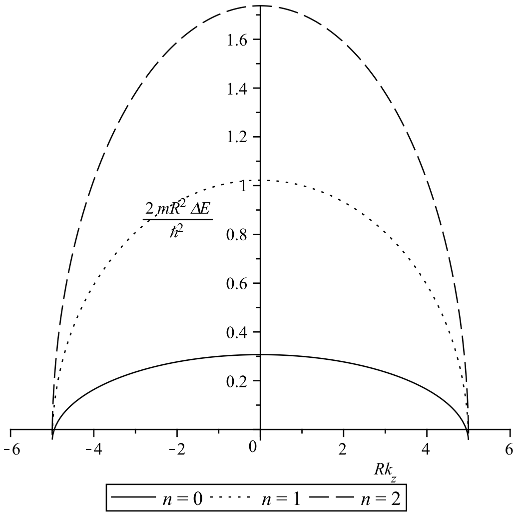

Figure 2: The energy difference, $\Delta \equiv \left|E'_n - E_n\right|$, between two models: one with and the other without the deformed potential. Δ versus Rk_z for $\alpha = 10$ and $\lambda = 0.4$. Notice the dispersion curves with maximum value at $k_z = 0$.

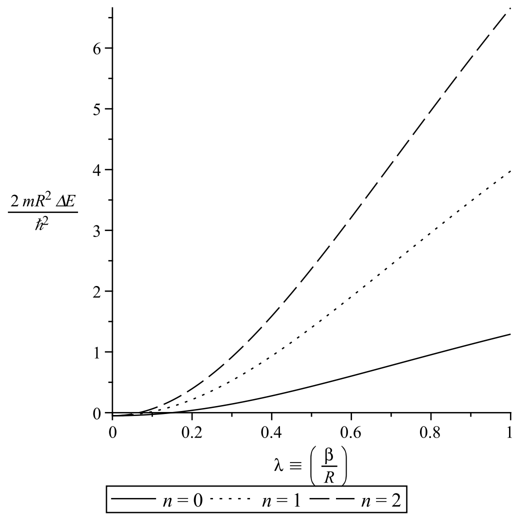

Figure 3: The energy difference, $\Delta \equiv \left|E'_n - E_n\right|$, between two models: one with and the other without the deformed potential. Δ versus the ratio between the Burges vector and the radius of the cylinder, $\beta/R = 1(\alpha = 10$ and $Rkz = 2)$. The energy difference is increased until $\beta/R = 1$.

a flat sample, it is well known that the Landau levels are linear with respect the magnetic field intensity. The dispersion due to curvature changes this fact. In Ref. [18], the energy spectrum and the ballistic transport of a 2DEG on a cylindrical surface were theoretically investigated. The authors investigated the hall conductivity in the case where only the lowest Landau band is occupied (ultra-quantum limit), the case when more than one

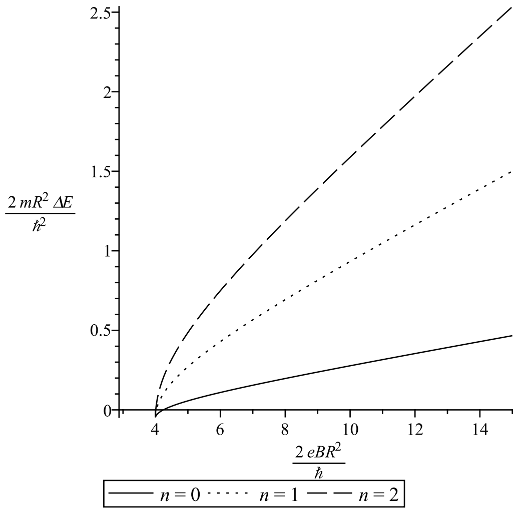

Figure 4: The energy difference, $\Delta \equiv \left|E_n' - E_n\right|$, between two models: one with and the other without the deformed potential. Δ versus $\alpha \equiv (2eBR^2)/\hbar$ for $Rk_z = 2$ and $\lambda = 0.4$. Δ is pronounced for higher magnetic fields. See that there is one value of the magnetic field to which $\Delta = 0$.

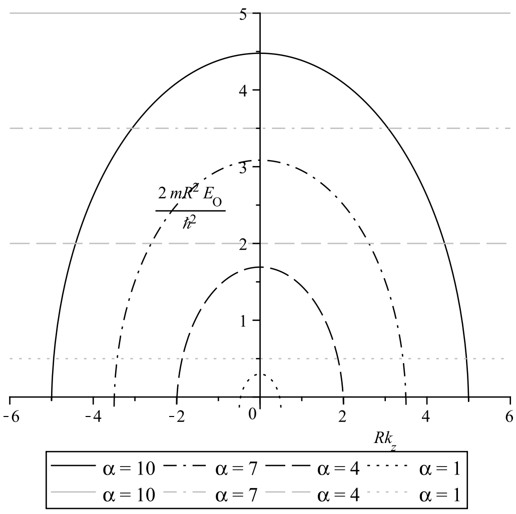

Figure 5: E_n versus Rk_z for different values of the magnetic field. The curves are also equally spaced and the maximum values of energy are lower than the Landau levels in a flat sample.

non-overlapping Landau bands are occupied and the case when more than one *overlapping* Landau bands are occupied. In order to appreciate the influence of a screw dislocation on such phenomenon, we consider just the ultra-quantum limit. To see the consequences in the other cases, one can just follow the Ref. [18]. We start by considering the existence of an electric field F which is supposed to be directed along the arc $[-\theta_0, \theta_0]$. We

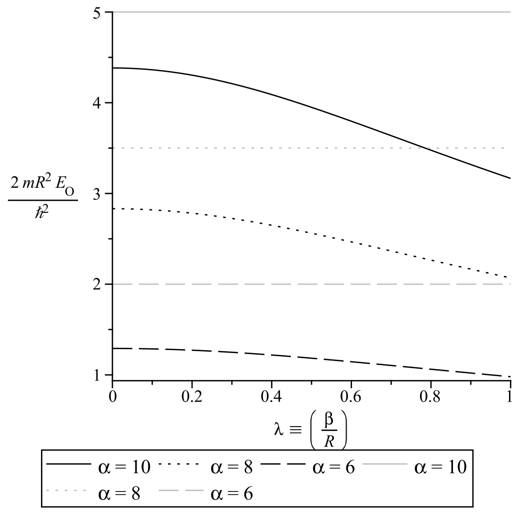

Figure 6: Plot of E_0 versus $\frac{\beta}{R}$(ratio between the Burger's vector and the cylinder radius), for different values of the magnetic field.

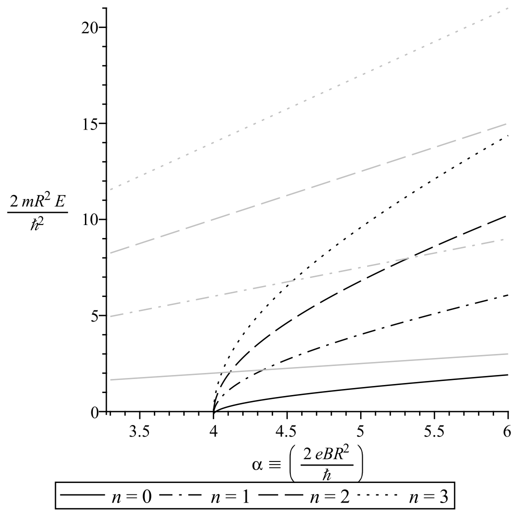

Figure 7: Energy levels as function of $\alpha \equiv \frac{2eB}{\hbar}R^2$ for $\lambda = 0.4$ and $Rk_z = 2$. Due to dispersion, these energies are no longer linear with respect the magnetic field.

must add the potential $eFr\theta$ in the Schrodinger equation (14). After expanding the effective potential in Eq. (14) up to the harmonic term around the minimum x_M, we rewrite the Eq. (16) as

$$\begin{aligned} E_n &= \left(n + \frac{1}{2}\right)\Omega - eFr\arcsin\left(\frac{\hbar k_Z}{eBr}\right) - \frac{e^2F^2}{2m\Omega^2} \\ &- \frac{\hbar^2}{8mR^2}\left(1 + \frac{\beta^2}{R^2}\right)^{-1} + \frac{\hbar^2}{m}\frac{\beta^2}{a^2R^2}, \end{aligned} \tag{19}$$

where

$$\Omega \equiv \hbar\omega_c \left(1+\frac{\beta^2}{R^2}\right)^{-\frac{1}{2}} \sqrt{1-\left(\frac{\hbar k_Z}{eBr}\right)^2}.$$

By defining $B' \equiv B/\left(1+\frac{\beta^2}{R^2}\right)^{\frac{1}{2}}$, we can rewrite the expression (19) as

$$\begin{aligned} E_n &= \left(n+\frac{1}{2}\right)\frac{\sqrt{1-\left(\frac{l_B'^2 k_z}{r}\right)^2}}{m l_B'^2} - eFr\arcsin\left(\frac{l_B'^2 k_z}{r}\right) \\ &- \frac{e^2F^2m^2 l_B'^4}{2m\left(1-\frac{l_B'^4 k_z^2}{r^2}\right)} - \frac{\hbar^2}{8mR^2}\left(1+\frac{\beta^2}{R^2}\right)^{-1} + \frac{\hbar^2}{m}\frac{\beta^2}{a^2R^2}. \end{aligned} \quad (20)$$

We evoke the result of the Hall conductivity on a cylinder without any defect which is found in Ref. [18], namely

$$G_H = G_0\left[1-\frac{\arcsin(\sin\phi_0 - \pi\phi_0 N_s l_B)}{\phi_0}\right], \quad (21)$$

which is valid for $\cos\phi_0 > 1/3$. In this expression, $G_0 \equiv 2e^2/h$ is the conductance quantum, $l_B^2 \equiv \hbar/eB$ and $N_s \equiv \left(m/2\pi\hbar^2\right)E_F$ is the electronic density. In the case with a screw dislocation, we make the changes $l_B^2 \to l_B'^2$, $\phi_0 \to \theta_0 \equiv \phi_0 + \beta z_0/\left(R^2\sqrt{1+\frac{\beta^2}{R^2}}\right)$ and

$$\begin{aligned} N_s &\to N_s' \\ &\equiv \frac{m}{2\pi\hbar^2}\left(E_F + \frac{\hbar^2}{8mR^2}\left(1+\frac{\beta^2}{R^2}\right)^{-1} - \frac{\hbar^2}{m}\frac{\beta^2}{a^2R^2}\right). \end{aligned} \quad (22)$$

Notice that the curvature potential and the contribution due to the deformed potential modify the electronic density. This was observed in the case of curvature only in Ref. [19].

For $\theta_0 << 1$, we have

$$G_H = \frac{N_s' e}{B'} + \frac{G_0\theta_0^2}{12}\left[1-\left(1-\frac{\nu'}{2}\right)^3\right], \quad (23)$$

Considering the expressions above and $z_0 = b$, the Hall conductivity can be ready as

$$\begin{aligned} G_H &= \frac{\frac{m}{2\pi\hbar^2}\left(E_F + \frac{\hbar^2}{8mR^2}\left(1+\frac{\beta^2}{R^2}\right)^{-1} - \frac{\hbar^2}{m}\frac{\beta^2}{a^2R^2}\right)e}{B\left(1+\frac{\beta^2}{R^2}\right)^{-\frac{1}{2}}} \\ &+ \frac{G_0\left(\phi_0 + 2\pi\frac{\beta^2}{R^2\sqrt{1+\frac{\beta^2}{R^2}}}\right)^2}{12}\left[1-\left(1-\frac{\nu'}{2}\right)^3\right], \end{aligned} \quad (24)$$

where $\nu' \equiv 2\pi N_s' l_B'^2$. From Fig. 8, we can see that the screw dislocation enhances the hall conductivity as the Burges vector is increased.

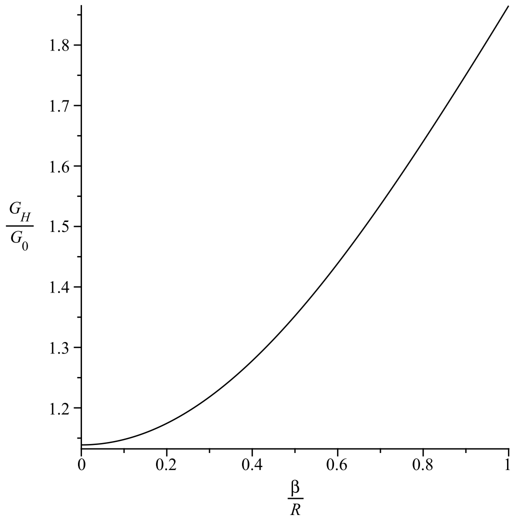

Figure 8: Enhancement of the Hall conductivity as $\frac{\beta}{R}$ is increased. We considered $l_B/R = 0.5$, $\phi_0 = 0.4\pi$ and $\frac{2mR^2E_F}{\hbar^2} = 2$.

4. Concluding Remarks

In conclusion, we studied the effect of a screw dislocation on the energy levels of a 2DEG confined on a cylindrical surface. We have considered the effects of two contributions: the covariant term which comes from the geometric approach in the continuum limit and a noncovariant repulsive scalar potential. Both appear due to elastic deformations on a semiconductor with such kind of topological defect. This case, showing such deformed potential can be thought in the context of 3D semiconductors where the electrons are confined on a cylindrical shell. The absence of this noncovariant potential could find place in the context of carbon nanotubes which are intrinsically two dimensional entities and such potential has not been derived. We have found that this noncovariant term changes significantly the energy levels of electrons in this system. In the absence of any magnetic field, the results can be explored in the context of quantum rings. When a constant external magnetic field is present, we observed significant modifications in the Landau levels and this will have important consequences in the Quantum Hall effect. In fact, the diminished effective frequency enhances the hall conductivity in the ultraquantum limit. In the other regimes, the steps of the Hall conductivity usually shift to higher magnetic fields in this case[20, 21]. The quantum Hall effect on a cylinder without any defect was investigate in reference [22] and it can be a start point if one has intention to evaluate deeply the influences of a screw dislocation is this phenomenon. Measurements of Hall conductivity in this particular geometry are provided in Refs. [23, 24]. Again, thermodynamical properties in such geometry without defects are theoretically investigated in [25].

As a final word, we remember the reader that we have investigated the 2DEG in the harmonic approximation, which is

valid for a sufficiently strong normal to the surface component of the magnetic field and for electrons with the Landau oscillator suspension center far enough from the side edges of a cylindrical strip. If higher terms in the Hamiltonian is to be take into account, the Ref. [16] can be used in order to treat the problem via the perturbation theory. The authors have done this, again, for a 2DEG on a cylinder without any kind of defect.

Acknowledgments

This work was supported by the CNPq, Brazil, Grants No. 482015/2013-6 (Universal), No. 476267/2013-7 (Universal), No. 306068/2013-3(PQ); FAPEMA, Brazil, Grant No. 00845/13 (Universal) and. project No. 01852/14 (PRONEM).

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